

Evaluation of the catalytic performance

The CO oxidation activity tests were evaluated in a fixed-bed quartz reactor using a U-shaped quartz tube with an inner diameter of 6 mm under the following typical reaction condition: $[\text{CO}] = 1 \text{ vol.}\%$, $[\text{O}_2] = 21 \text{ vol.}\%$, N_2 as balance gas with a total flow rate of 30 mL min^{-1} , and the catalyst mass for each test is 50 mg. GC9310 gas chromatograph (equipped with a TDX-01 column and a TCD detector) and N-2000 workstation were used for collecting and analyzing the reactants and products. The conversion of CO (X_{CO}) was calculated using eq.:

$$X_{\text{CO}} = \left(1 - \frac{S_{\text{CO-outlet}}}{S_{\text{CO-inlet}}}\right) \times 100\% \quad (\text{S1})$$

where $S_{\text{CO-outlet}}$ and $S_{\text{CO-inlet}}$ are the CO concentration in the inlet and outlet gas streams corresponding to the CO inlet and outlet peak areas, respectively, which derived from the gas chromatograph responses using modified area normalization method.

DFT Calculations

During adsorption calculations, a kinetic energy cutoff of 500 eV was used. A gamma-centered $1 \times 1 \times 1$ mesh was employed for Brillouin zone integration. Geometry optimization was performed using the whole molecule model relaxation. A vacuum layer with a thickness of at least 20 Å in the z -direction was added to simulate surfaces and ensure that the reaction was not influenced by the next layer. The convergence criteria for electronic and geometry relaxation were set to 10^{-5} eV and $0.01 \text{ eV} \cdot \text{\AA}^{-1}$, respectively. Adsorption was allowed on only one side of the exposed surface, and the dipole moment was corrected in the z -direction. The adsorption energy (E_{ads}) of reaction gas on the Fe_2O_3 (101) surface was calculated using Equation (S2):

$$E_{\text{ads}} = E_{\text{gas-structure}} - (E_{\text{gas}} + E_{\text{structure}}) \quad (\text{S2})$$

where E_{ads} , $E_{\text{structure}}$, and E_{gas} are the total energies of adsorbed reaction gas over the SnO_2 (110) surface, interacting SnO_2 (110) structure surface, and isolated gas molecules in a vacuum, respectively.

The reaction energy (E_r) was defined as Equation (S3):

$$E_r = E_{\text{FS}} - E_{\text{IS}} \quad (\text{S3})$$

where E_{IS} and E_{FS} are the energies of the initial and final states, respectively.

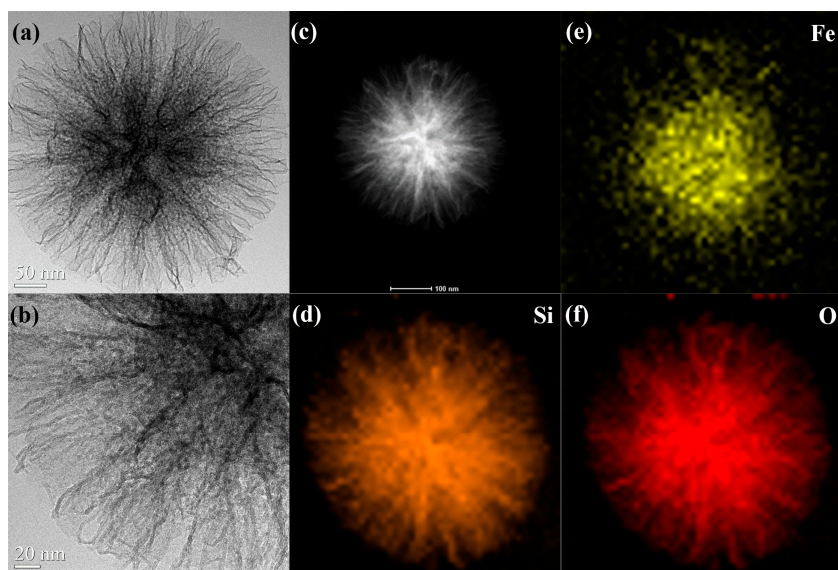


Figure S1. (a, b) TEM, (c-f) HAADF-STEM and Mapping images of 7%Fe@KCC-1 catalysts.

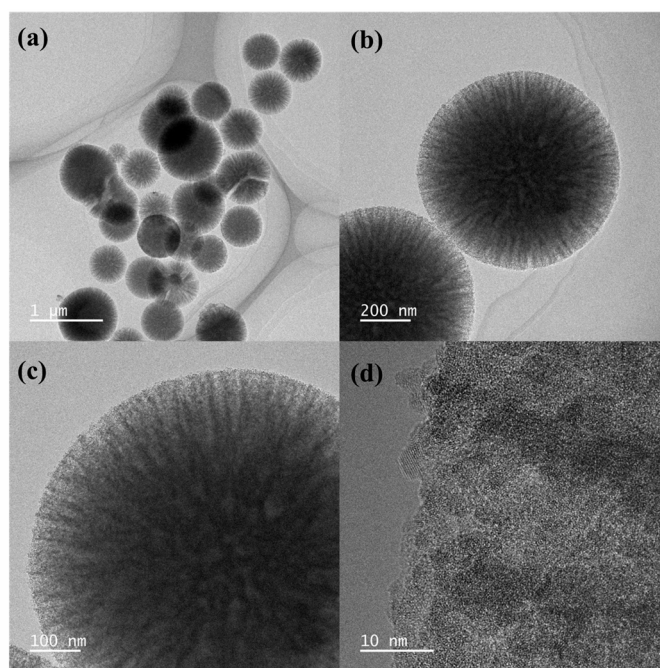


Figure S2. (a-d) HRTEM for reduced 7%Fe@KCC-1 catalyst by H₂.

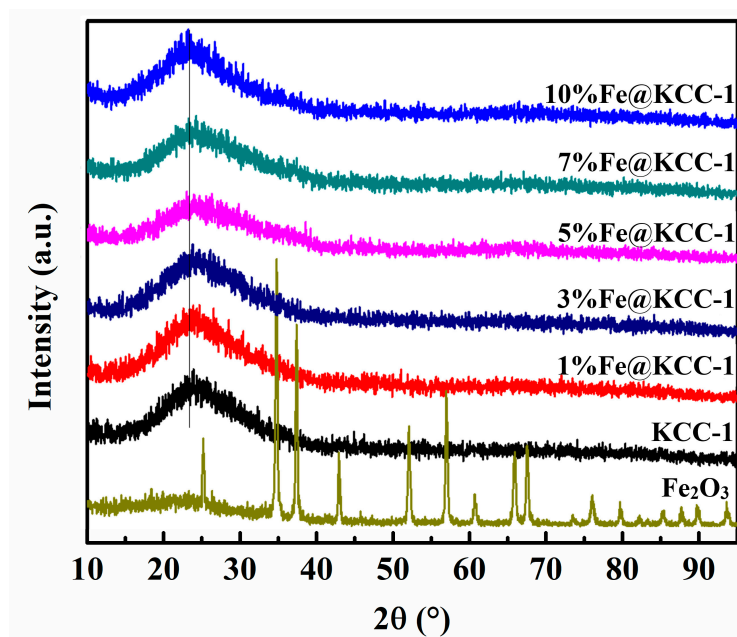


Figure S3. XRD patterns of $x\%$ Fe@KCC-1 ($x=0, 1, 3, 5, 7$ and 10) and related catalyst materials.

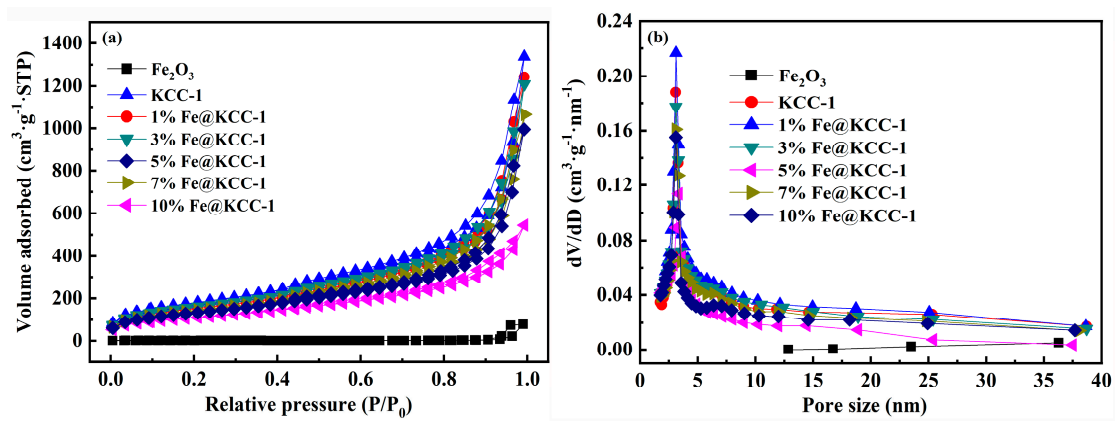


Figure S4. (a) N_2 adsorption-desorption isotherms and (b) pore size distribution curves of $x\%\text{Fe@KCC-1}$ ($x=0, 1, 3, 5, 7$ and 10) and related catalyst materials.

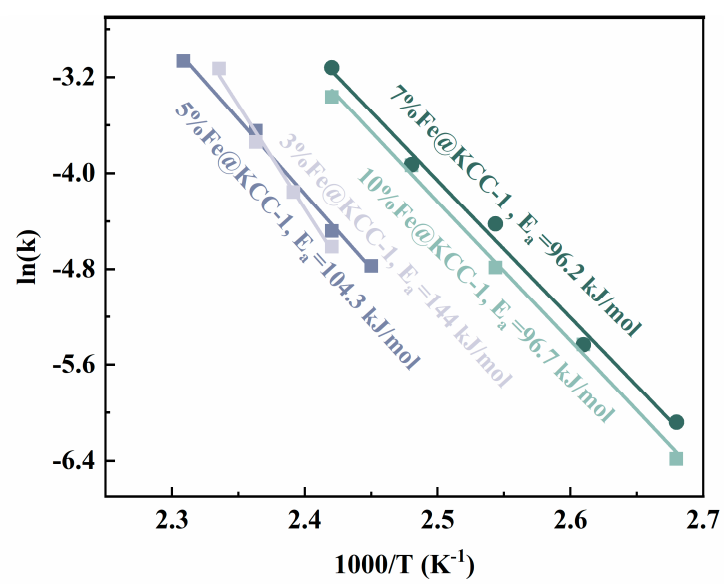


Figure S5. Arrhenius plots for CO oxidation over different catalysts.

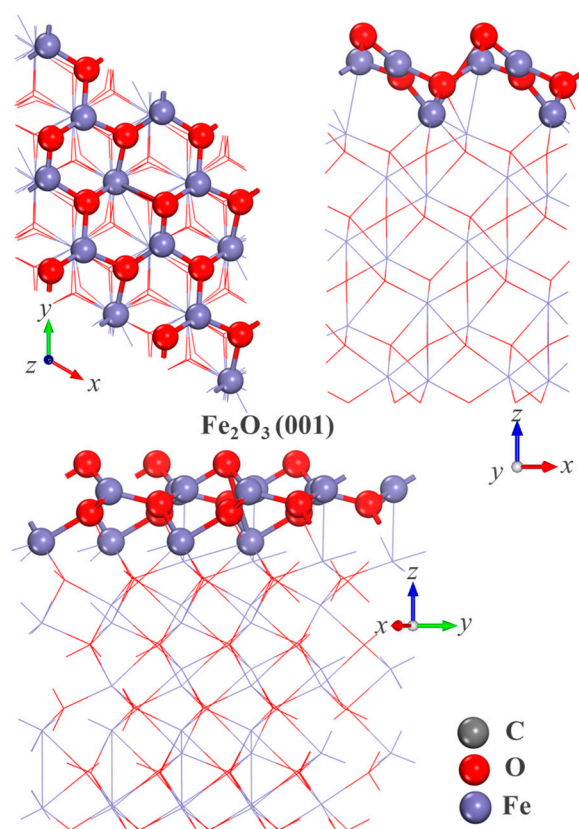


Figure S6. Top and side view of the optimized Fe_2O_3 (001) catalyst structure.